

Critical wave functions in disordered graphene

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In order to elucidate the presence of non-localized states in doped graphene, an scaling analysis of the wave function moments known as inverse participation ratios is performed. The model used is a tight-binding hamiltonian considering nearest and next-nearest neighbors with random substitutional impurities. Our findings indicate the presence of non-normalizable wave functions that follow a critical (power-law) decay, which are between a metallic and insulating behavior. The power-law exponent distribution is robust against the inclusion of next-nearest neighbors and on growing the system size.

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Graphene is a two-dimensional atomic crystal [1] with the highest known charge carrier mobility [2] and thermal conductivity [3] at room temperature. Both properties set up graphene as a raw material for transistors, however, the ‘*graphenium inside*’ era is quite far [4]. Keeping in mind the aim of design a transistor, the problem turns out to be how to alchemize it into a semiconductor. An alternative is to dope graphene. This leads immediately to the question of having quantum percolation in two dimensions, which has been the subject of debate many years ago [5, 6]. In the literature, usually it is found that “there is no true metallic behavior in two dimensions” as a consequence of the fact that all eigenstates are localized even when the disorder is weak [7]. In graphene, there has been a debate about this point [8–10]. Recently, disordered graphene has been classified using symmetry arguments around the Dirac point [11]; this classification allows a minimal conductivity behavior. Experimentally, the minimal-conductivity was measured for potassium atoms onto the graphene surface [12, 13]. Furthermore, it has been found that a metal-transition can be observed when graphene is doped with H [14]. Also, using a non-interacting electron model enriched by first-principles calculation the metal-insulator transition is observed [15, 16]. In this Letter, we present numerical evidence that shows a very interesting scenario. We have characterized the probability distribution of the moments associated to the wave function using the inverse participation ratios. The scaling of this quantity is frequently used to discriminated when an eigenstate is extended or localized. In doped graphene, we found extended states which do not follow the usual exponential localization; instead, these are critical,

i.e., the wave function decay spatially as a non-normalizable power-law. This behavior evidenced the multifractality of the wave function [17]. Notice that in the original development of the scaling theory, critical states were not considered [7].

As a model we use the tight-binding hamiltonian,

$$\mathcal{H} = -t \sum_{\langle i,j \rangle} c_i^\dagger c_j - t' \sum_{\langle\langle i,j \rangle\rangle} c_i^\dagger c_j + \varepsilon \sum_{\ell} c_{\ell}^\dagger c_{\ell}, \quad (1)$$

where the nearest neighbor, $t = 2.79$ eV, and next-nearest neighbor (NNN), $t' = 0.68$ eV, hopping parameters are included; these values have been taken from reference [18]. The impurity sites, ℓ , have been distributed randomly in the lattice according with a fixed concentration, C ; and ε is the self-energy for an impurity.

In order to investigate localization, we introduce the inverse p-participation ratios (IPRs),

$$||\Psi_{\mathbf{k}}||_{2p} = \sum_i^N |\Psi_{\mathbf{k}}(\mathbf{r}_i)|^{2p}, \quad (2)$$

where $\Psi_{\mathbf{k}}$ is the wave function associated to the eigenstate \mathbf{k} with energy $E_{\mathbf{k}}$, which solves the Schrödinger equation $\mathcal{H}\Psi_{\mathbf{k}} = E_{\mathbf{k}}\Psi_{\mathbf{k}}$. The index i belongs to the sum over sites, N is the total number of sites and p is an integer. When $p = 1$, $||\Psi_{\mathbf{k}}||_2 = 1$ because of the normalization condition. If the wave function of the eigenstate follows the power-law, $\Psi(\mathbf{r})_{\mathbf{k}} \sim |\mathbf{r}|^{-\alpha}$, the p-IPRs are scaled as [19],

$$||\Psi_{\mathbf{k}}||_{2p} \simeq \begin{cases} N^{-(p-1)} & (0 \leq \alpha < \frac{1}{p}) \\ N^{-p(1-\alpha)} & (\frac{1}{p} \leq \alpha < 1), \\ N^0 & (1 \leq \alpha) \end{cases}, \quad (3)$$

when $p > 1$. The behavior N^{-1} corresponds to a metal while N^0 corresponds to an insulator. Notice that here $N \propto L^2$, where L it is the length sample.

To evaluate Eq. (2), we calculated all the eigenvalues and eigenvectors of \mathcal{H} by numerical diagonalization. The $p = 2$ IPR behavior is shown in Figure 1 as a function of N for several selected energies, using different impurities self energies without and with NNN interaction. For the energy $E_e = E_D - 0.4t$, far from the Dirac energy, we compare the behavior for pure graphene [(green online) diamonds] with doped graphene [(blue online) squares]. For pure graphene, the state is extended since the $p=2$ IPR goes like N^{-1} , as shown in Figure 1. For doped graphene, is clear that the $p=2$ IPR can be fitted with a line, which suggests a non-localized, power law behavior. On the other hand, for states near the Dirac energy, in doped graphene the (dark blue online) circles and (red online) triangles behavior suggests localized states, since the $p=2$ IPR scales as $\propto N^0$. Thus, from this scaling analysis is clear that doped graphene, even in the absence of NNN interaction, presents different kinds of localization, as has been suggested in reference [20] due to frustration effects [21], as well as in experiments [14].

In order to know the exponent distribution of the power law behavior, we introduce the integrated distribution of exponents [19],

$$I(\gamma) = \frac{1}{N} \sum_{E_k} \Theta \left(\gamma - \log_N [||\Psi_{E_k}||_8] \right), \quad (4)$$

where Θ is the step function. The exponent distribution is plotted in Figure 2 for several impurity types and two different concentrations, 1% and 5%. For pure graphene, all the states have the same scaling behavior, and a step is observed at $\gamma = -3$. This means that all states have the same scaling, and thus all are extended, as expected from Bloch's theorem. However, for doped graphene, we observe two main effects. First there is a shift to higher values of γ and second, the jump is not anymore a discontinuity. Instead, we observe states that have a distribution of γ values. In all cases, we observed that the minimal value of γ is $\approx -5/2$, which means that the most extended states, follow a power law that goes as $r^{-3/8}$. States with $\gamma \approx 0$ are exponentially localized. Since no clear jump is observed in the values of γ , it seems that there is a range of values for the exponents of the critical wave functions. Also, it is worthwhile mentioning that the presence of the NNN interaction preserves this behavior, which al-

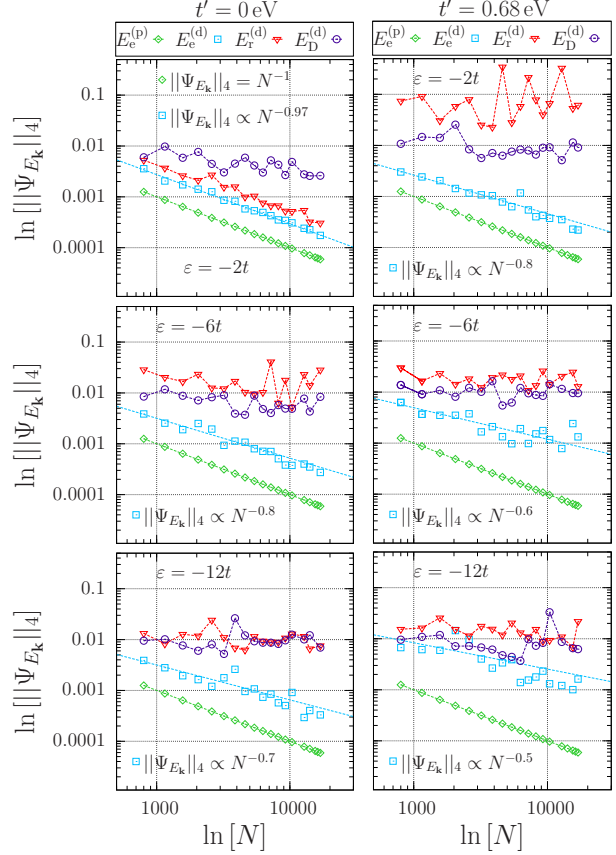


FIG. 1. (Color online) The $p = 2$ IPR behavior as a function of N for several selected energies, using different impurities self energies (from top to bottom) and without and with NNN interaction (left and right columns, respectively). The selected energies are the Dirac point energy [E_D , (dark blue online) circles], the resonant state energy [E_r , (red online) triangles] and $E_e = E_D - 0.4t$ [(blue online) squares] for doped graphene ^(d). In all cases, doped graphene has a 5% impurity concentration. For the state with energy E_e , we present in all cases the scaling exponent that results from the fitting, shown in the figures with (blue online) lines. For comparison proposes, we include the case of pure graphene for the energy $E_e^{(p)}$ [(green online) diamonds].

lows its experimental verification since the NNN is always present.

To verify that such behavior is preserved as the system grows, in Fig. 3 we present the distribution $I(\gamma)$ for different sample sizes. We can observe that the behavior is very similar at all sizes. From this analysis, we can conclude that there are many non-exponentially localized states, and that the power law behavior is not a finite size lattice effect. From

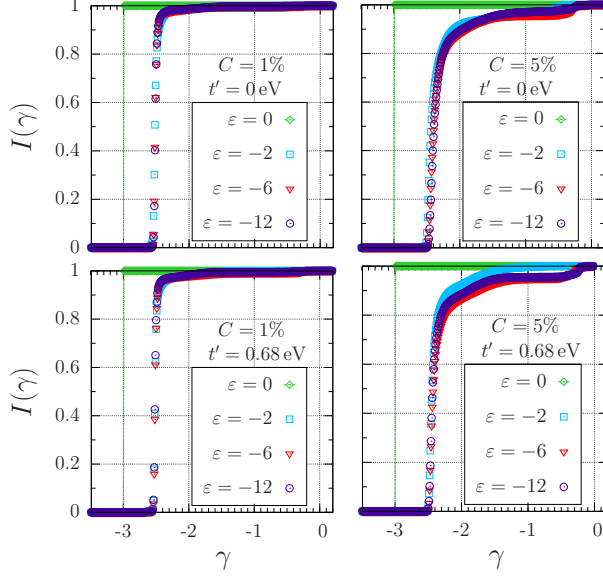


FIG. 2. (Color online) Integrated distribution of exponents for different impurity configurations using lattices with $N = 16,928$ sites. Extended states are at $\gamma = -3$ and localized at $\gamma = 0$. We observe that for pure graphene [(green online) diamonds], the distribution is a step function at $\gamma = -3$, meanwhile for doped graphene the distribution is shifted and it is no longer a step function.

the values of γ , these states are critical and non-normalizable. Finally, a careful check of such states reveals that localized states are near the Dirac point and at the band edges, while the power law non-normalizable states are near the middle part of the valence and conduction band, in agreement with previous theoretical arguments [20, 21].

In conclusion, using a scaling analysis of the participation ratio, we have shown that the presence of disorder in graphene do not localize exponentially all states; instead, some states are critical with a distribution of exponents. This result is robust against the inclusion of NNN interactions, in which the chirality is not preserved. This result is not only important for graphene, but it makes a revival of an old discussion concerning the possibility of having anomalous quantum percolation in two dimensional systems [5, 6].

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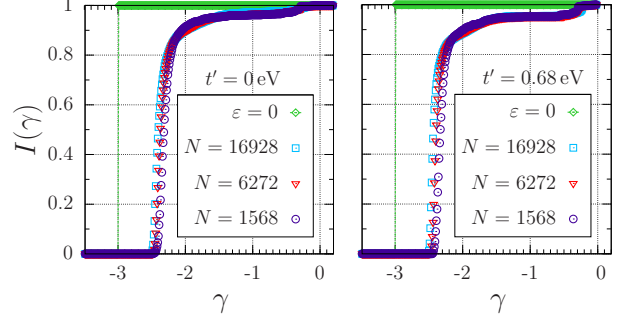


FIG. 3. (Color online) Example of the Integrated distribution of exponents for different sample sizes using a fixed concentration of impurities (5%) with self-energy $\varepsilon = -6t$. The left panel corresponds to the model without NNN interaction, and the right panel graph with NNN.

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